Algorithm for Reconstructing 3D-Binary Matrix with Periodicity Constraints from Two Projections

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Abstract—We study the problem of reconstructing a three dimensional binary matrices whose interiors are only accessible through few projections. Such question is prominently motivated by the demand in material science for developing tool for reconstruction of crystalline structures from their images obtained by high-resolution transmission electron microscopy. Various approaches have been suggested to reconstruct 3D-object(crystalline structure) by reconstructing slice of the 3D-object. To handle the ill-posedness of the problem, a priori information such as convexity, connectivity and periodicity are used to limit the number of possible solutions. Formally, 3D-object(crystalline structure) having a priory information is modeled by a class of 3D-binary matrices satisfying a priori information. We consider 3D-binary matrices with periodicity constraints, and we propose a polynomial time algorithm to reconstruct 3D-binary matrices with periodicity constraints from two orthogonal projections.

Keywords—3D-Binary Matrix Reconstruction, Computed Tomography, Discrete Tomography, Integral Max Flow Problem.

I. INTRODUCTION

THE area of *discrete tomography* is concerned about reconstruction of a discrete object or its geometrical properties from its projections or some other information. This has application in fields such as: computer vision, VLSI design, image processing [12], statistical data security [9], biplane angiography [11], graph theory, crystallography, medical imaging [7] etc. [5] gives the fundamentals related to this topic.

Peter Schwander and Larry Shepp proposed a model that identifies each possible atom location with a cell of integer lattice Z^3 and the electron beams with lines parallel to given direction. The value 1 in a cell of Z^3 denotes the presence of atom in the corresponding location of crystal and the value 0 in a cell of Z^3 denotes the absence of atom in the corresponding location of the crystal. The number of atoms that are present in the line passing through the crystal defines the projection of the structure along the line [10]. The set of all projections of structure along each line parallel to given direction denotes one projection of the object. The number of atoms present in a line(straight) can be computed by making quantitative analysis of two-dimensional images taken by the transmission electron microscope. The transmission electron microscope uses high energy rays which penetrates the crystal. Hence to get more projections, large amount of energy is to be transmitted through the crystal, which can damage the crystal itself(the atomic configuration may be changed). The conventional *Computed Tomography* needs

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more projections(usually hundreds of projections) for effective reconstruction of the objects. *Discrete Tomography* considers the case where the objects need to be reconstructed with few projections(usually two to four).

As crystal is represented by binary matrix, reconstructing crystal is same as reconstructing 3D-binary matrix. 3D-binary matrix can be reconstructed by slice-by-slice reconstruction. Hence the problem of reconstructing 3D-binary matrix is reduced to reconstructing 2D-binary matrix. Reconstructing 2D-binary matrix was studied much before the emergence of its practical application. In 1957 Ryser [8] and Gale [3] gave a necessary and sufficient condition for a pair of vectors being the projections of binary matrices along horizontal and vertical directions. The projections in horizontal and vertical directions are equal to row and column sums of the matrix. They have also given necessary and sufficient conditions for existence of unique 2D-binary matrix which has a given pair of row sum and column sum. In general, the class of binary matrices having same row and column sums is very large. Though the reconstructed matrix and the original matrix have same projections, they may be very different. One of the main issues in *Discrete Tomography* is to reconstruct the object which is more close to the original object with few projections only. One approach to reduce the class of possible solutions is to use some a priori information about the objects. For instance, convex binary matrices have been reconstructed uniquely from projections taken in some prescribed set of four directions in [4]. An another approach is given in [6], where the class of binary matrices having same projections is assumed to have some Gibs distribution. By using this information, object which is close to the original unknown object is reconstructed.

We consider the first approach, periodicity in particular, to limit the possible solutions of 3D-Binary matrices having given projections. Similar approach has been suggested in [1]. In [1], some variance of 2D-periodic-binary matrices are reconstructed in polynomial time. Those algorithms can be used to reconstruct 3D-binary matrices in which periodicity lies with in the slice(not across the slices). In general, periodicity structure need not be restricted to within slice. So we consider the reconstruction of 3D-binary matrix with periodicity constraints not restricted to within slice.
In this paper, we introduce some variance of 3D-binary matrices with periodicity constraints and we give a polynomial time algorithm for reconstructing one variant of 3D-binary matrix with periodicity from two orthogonal projections(projections along X and Y or Y and Z or X and Z axes). We leave other variants of this problems open.

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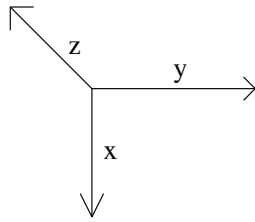International Journal of Computer and Information Engineering
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Fig. 1.   Orientation of 3D-Matrix

II. NOTATIONS AND DEFINITIONS

Let $A^{l \times m \times n} = (a_{i,j,k})$ be a 3D-binary matrix of order $l \times m \times n$, where $1 \le i \le l$, $1 \le j \le m$, $1 \le k \le n$. Let $X = (x_{j,k})$ and $Y = (y_{i,k})$ be orthogonal projections along the axes x and y respectively, where

$$x_{j,k} = \sum_{i=1}^{n} a_{i,j,k} \qquad y_{i,k} = \sum_{j=1}^{m} a_{i,j,k}$$

and $1 \le i \le l$, $1 \le j \le m$ and $1 \le k \le n$. A 3D-binary matrix $A^{l \times m \times n} = (a_{i,j,k})$ is said to be (p,q,r)-periodic if $a_{i,j,k} = a_{i+p,j+q,k+r}$ where $1 \le i+p \le l$, $1 \le j+q \le m$, $1 \le k+r \le n$.

Example 1: A (1,1,1)-periodic matrix and its two orthogonal projection matrices are given bellow(We use layer by layer representation of 3D-binary matrix with the orientation given in Fig 1.).

3D-binary matrix (layer-by-layer representation) A:

$$
\begin{bmatrix} 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 1 & 0 \end{bmatrix}
\begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 \end{bmatrix}
\begin{bmatrix} 1 & 1 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 \end{bmatrix}
$$

$$
\begin{bmatrix} 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix}
$$

Projection matrices of A:

$$Y = \begin{bmatrix} 2 & 1 & 3 & 3 \\ 3 & 2 & 1 & 3 \\ 3 & 3 & 2 & 2 \\ 3 & 2 & 2 & 2 \end{bmatrix}$$

and

$$X = \begin{bmatrix} 3 & 3 & 3 & 2 \\ 1 & 2 & 2 & 3 \\ 2 & 2 & 1 & 3 \\ 4 & 3 & 1 & 2 \end{bmatrix}$$

where Y and X are projections of given matrix A along y and x axes respectively.

For any given triple (x,y,z) such that $a_{x,y,z} = 1$ we define the set P of propagation of the value in position (x,y,z) in the direction (p,q,r),
$P = \{(x+kp, \; y+kq, \; z+kr)| \; 1 \le x+kp \le l, \; 1 \le y+kq \le m, \; 1 \le z+kr \le n, \; k \in Z\}$. Such set is called

as line. Each line has a *starting point*, which is its left most point, and an *ending point* , which is rightmost point. We say a line starts on column j in layer k and ends on column j' in layer k' when its starting and ending points are on column j in layer k and column j' in layer k' respectively.

Let A be a (p,q,r)-periodic matrix. From periodicity it follows that if there exists indices $1 \le i \le l$ and $1 \le k \le n$ such that $y_{i,k} = y_{i+p,k+r} + a$ where $1 \le i+p \le l$, $1 \le k+r \le n$, then the positions on row i and layer k, from column $m-q+1$ to column m, contains at least a elements equal to 1. Such positions form a box at right end of the row i , and the box is called as *right box(rt)* $y_{i,k} + a = y_{i+p,k+r}$ where $1 \le i+p \le l$, $1 \le k+r \le n$, then the positions on row $i+p$ and layer $k+r$, from column 1 to column q, contains at least a elements equal to 1. Such positions form a box at left end of the row $i+p$, and the box is called as *left box(rt)*.

We define the upper and lower boxes as follows: If there exists indices $1 \le j \le m$ and $1 \le k \le n$ such that $x_{j,k} = x_{j+q,k+r} + a$ when $1 \le j+q \le m$, $1 \le k+r \le n$, then the positions on column j and layer k, from row $l-p+1$ to row l, contains at least a elements equal to 1. Such positions form a box at end of the column j , and the box is called as *lower box(lw)*, and if $x_{j,k} + a = x_{j+q,k+r}$ where $1 \le j+q \le m$, $1 \le k+r \le n$, then the positions on column $j+q$ and layer $k+r$, from row 1 to row p, contains at least a elements equal to 1. Such positions form a box at beginning of the column $j+q$, and the box is called as *upper box(up)*

We define diagonally homogeneous and strongly diagonally homogeneous 2D-matrices as follows. A 2D-matrix $M = (m_{i,j})$ is said to be (a, b)-diagonally homogeneous if $m_{i, \; j} = m_{i+a, \; j+b} \; for \; all \; 1 \le i+a \le l$, $1 \le j+b \le m$. A 2D-matrix $M = (m_{i,j})$ is said to be (a, b)-strongly diagonally homogeneous if M is diagonally homogeneous and
for all $1 \le i+a \le l$, $m-b+1 \le j \le m$, $m_{i, \; j} = m_{i+a, \; (j+b)mod \; m}.$

III. RECONSTRUCTION OF (1,1,1)-PERIODIC MATRIX

In this section, we give an algorithm to reconstruct a (1,1,1) periodic matrix of size $n \times n \times n$ from two orthogonal projections.

Let A be a (1,1,1)-periodical matrix. By definition of boxes for $p = 1$, $q = 1$ and $r = 1$ the boxes are reduced to only one cell and the integer a of the definition takes only the values 0 or 1. if there exists indexes $1 \le i+1 \le n$ and $1 \le k+1 \le n$ or $1 \le j+1 \le n$ and $1 \le k+1 \le n$ such that
$y_{i,k} = y_{i+1,k+1} + 1$ then $a_{i,m,k} = 1$.
$y_{i,k} + 1 = y_{i+1,k+1}$ then $a_{i+1,1,k+1} = 1$.
$x_{j,k} = x_{j+1,k+1} + 1$ then $a_{j,l,k} = 1$.
$x_{i,k} + 1 = x_{j+1,k+1}$ then $a_{j+1,1,k+1} = 1$.

We define the common portion of all matrices whose projections are same as given projections as *Fixed part* and the remaining portion of the matrix as *Mobile part* The following *Fixed part* algorithm uses the previous box properties to extract the fixed part(called F) of the reconstructed matrix. The following algorithm takes

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orthogonal projection matrices pair (X, Y) and gives the fixed part of the reconstructed matrix (namely the matrix F) and a pair of matrices (X', Y') that are projections of only mobile part of the reconstructed matrix.

Algorithm: $Fixed\ part$ Reconstruction
Input: A pair of integral matrices (X, Y) where $X = (x_{j,k})$ and $Y = (y_{i,k})$ are projection of 3D-binary matrix along x and y axes respectively.
Output: If $flag = 0$, then it gives the matrix (Fixed part) F and a pair of integral matrices (projections of the mobile part) (X', Y') or if $flag = 1$, then Failure in the reconstruction;
Initialization: $flag := 0$, $t := 0$, $X^t := X$, $Y^t := Y$, $F := 0^{l \times m \times n}$;

while X^t and Y^t are positives and diagonally
    non homogeneous matrices and $flag = 0$ **do**
    while Y^t is positive and diagonally non homogeneous
        matrix and $flag = 0$ **do**
        $X^{t+1} := X^t$, $Y^{t+1} := Y^t$
        for all indexes $1 \leq i, k \leq n$
          such that $y^t_{i,k} \neq y^t_{i+1,k+1}$;
          if $y^t_{i,k} = y^t_{i+1,k+1} + 1$ then
            $x := i$, $y := n$, $z := k$,
            Propagation(x, y, z, F, t)
          else if $y^t_{i,k} + 1 = y^t_{i+1,k+1}$ then
              $x := i+1$, $y := 1$, $z := k+1$,
              Propagation(x, y, z, F, t)
            else $flag := 1$;
          $t := t+1$;
    end while;
    while X^t is positive and diagonally non homogeneous
        matrix and $flag = 0$ **do**
        $X^{t+1} := X^t$, $Y^{t+1} := Y^t$
        for all indexes $1 \leq i, k \leq n$
          such that $x^t_{j,k} \neq x^t_{j+1,k+1}$;
          if $x^t_{j,k} = x^t_{j+1,k+1} + 1$ then
          $x := n$, $y := j$, $z := k$,
          Propagation(x, y, z, F, t)
          else if $x^t_{j,k} + 1 = x^t_{j+1,k+1}$ then
            $x := 1$, $y := j+1$, $z := k+1$,
            Propagation(x, y, z, F, t)
          else $flag := 1$;
          $t := t+1$;
    end while;
end while;
$X' = X^t$, $Y' = Y^t$ and return (X', Y').

Algorithm: Propagation(x, y, z, F, t)
  $P = \{(x+r, y+r, z+r) \mid 1 \leq x+r \leq n,$
    $1 \leq y+r \leq n, 1 \leq z+r \leq n, r \in Z\}$
  For all ($i, j\ k$) $\in P$ **do**
    $f_{i,j,k} := 1$, $x^{t+1}_{j,k} := x^t_{j,k} - 1$, $y^{t+1}_{i,k} := y^t_{i,k} - 1$;

Algorithm: $Make\_strong\_homogeneous$
Input: The matrix F and diagonally homogeneous matrices (X', Y')

Output: diagonally strong homogeneous matrices (X, Y)

Initialization: $X := X'$, $Y := Y'$;
    for all $1 \leq i \leq n$ **do**
        if $(y_{i,n} < y_{i+1,1})$
          $Propagation(i+1, 1, 1, F, t)$
        if $(y_{i,n} > y_{i+1,1})$
          $Propagation(i, n, n, F, t)$

Algorithm: $loop(x, y, z)$
  $P = \{(x', y', z') \mid x' := (x + r)mod\ n\ when\ (x + r)mod\ n \neq 0,\ otherwise\ n,$
  $y' := (y+r)mod\ n\ when\ (y+r)mod\ n \neq 0,\ otherwise\ n,$
  $Z' := (z + r)mod\ n\ when\ (z + r)mod\ n \neq 0,\ otherwise\ n,\ r \in Z\}$
  If there exists (i, j, k) $\in P$ **such that**
    $a_{i,j,k} = 1$, or $x_{j,k} = 0$ or $y_{i,k} = 0$, return 0, otherwise return 1.

Theorem 1: Let X and Y be the projections of unknown $(1,1,1)$-periodic matrix A of order ($n \times n \times n$) along x and y directions, F be the fixed part of A, F_x and F_y be the orthogonal projections of F along x and y axes respectively, and $X' = X - F_x$, $Y' = Y - F_y$. If X' and Y' are strongly diagonally homogeneous, then there exist a binary matrix M(mobile part) such that $A' = F + M$ and the projections of A are same as the projections of A' along x and y directions.
Proof. Let $G = (V_1, V_2, E)$ be a bipartite graph where $V_1 = \{d_i \mid 1 \leq i \leq n\}$ and $V_2 = \{d'_i \mid 1 \leq i \leq n\}$, and $E = \{(d_i, d'_j) \mid loop(1, j+i-1, i) = 1\}$.
Corresponding to G, We define a network $G' = (V, E', C)$. where $V = V_1 \cup V_2 \cup \{s,t\}$. $E' = E \cup \{(s,v) \mid v \in V_1\} \cup \{(v,t) \mid v \in V_2\}$.
$C(u,v) = 1$ if $u \in V_1$ and $v \in V_2$
for each $1 \leq i \leq n$, $C(s, d_i) = y_{1,i}$ $C(d'_i, t) = x_{1,i}$
Let f be a flow function whose net flow is maximum.
Let us construct $M = (m_{i,j,k})$ where $1 \leq i, j \leq n$ as follows:
Initialize M with zero matrix.
$m_{1,i+j-1,i} = 1$ if $f(d_i, d'_j) = 1$,
For each (i, j, k) $\in P = \{(x', y', z') \mid x' := (1+r)mod\ l\ when\ (1+r)mod\ l \neq 0,\ otherwise\ n,$
$y' := (i+j-1+r)mod\ n\ when\ (i+j-1+r)mod\ n \neq 0,\ otherwise\ n,$
$Z' := (i + r)mod\ n\ when\ (i + r)mod\ n \neq 0,\ otherwise\ n,\ r \in Z\}$, $m_{i,j,k} = 1$.
Let us define $A' = F + M$. By the definition of E and E', for every edge (d_i, d_j) such that $f(d_i, d_j) = 1$ a loop can start from $(1, j+i-1, i)$. Clearly all the loops corresponding to edges with flow value 1 are disjoint. By the definition of $loop()$, no loop corresponds to an edge will intersect with fixed part. Hence A' is a binary matrix. By the construction of M, projection of M along x and y axes are X' and Y' respectively. Hence projections of A' are same as projections of A along x and y.

Algorithm: $Mobile\ part$ Reconstruction
Input: The matrix F and a pair of integral matrices (X', Y')

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Output: If $flag1 = 0$, then it gives the matrix $A = F + M$, where M is mobile part. If $flag1 = 1$, then Failure in the reconstruction;

Initialization: $flag1 := 0$, $X := X'$, $Y := Y'$, $A := F$;

    Step1: Construct graph G and the corresponding network G' as defined in $Theorem 1$ for the projection matrices X and Y.

    Step2: Compute the flow function f for the net work G' using integral max flow algorithm.

    Step3: Compute sub graph $S = \{(d_i, d_j)' | f(d_i, d'_j) = 1\}$ of G'

    Step4: for every edge $(d_i, d'_j) \in S$ **do**
        $loop\_reconstruction(1, \ j + i - 1, \ i, \ A)$

    Step5: return $A = (a_{i,j,k})$

  Algorithm: $loop\_reconstruction(x, \ y, \ z, \ A, \ )$

    Step1: Compute $P = \{(x', \ y', \ z') \ | \ x' := (x + r) mod \ n \ when \ (x + r) mod \ n \neq 0, \ otherwise \ l,$
$y' := (y + r) mod \ n \ when \ (y + r) mod \ n \neq 0, \ otherwise \ n,$
$Z' := (z + r) mod \ n \ when \ (z + r) mod \ n \neq 0, \ otherwise \ n, \ r \in Z\}$

    Step2: For all $(i, \ j, \ k) \in P$ **do**
        $a_{i,j,k} := 1, \ x_{j,k} := x_{j,k} - 1, \ y_{i,k} := y_{i,k} - 1;$

EXAMPLE 2:

The above algorithm is illustrated with an example,
Input:

$$Y = \begin{bmatrix} 2 & 1 & 3 & 3 \\ 3 & 2 & 1 & 3 \\ 3 & 3 & 2 & 2 \\ 3 & 2 & 2 & 2 \end{bmatrix} \ and \ X = \begin{bmatrix} 3 & 3 & 3 & 2 \\ 1 & 2 & 2 & 3 \\ 2 & 2 & 1 & 3 \\ 4 & 3 & 1 & 2 \end{bmatrix}$$

Initialization: F :

$$\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

Make Y as diagonally homogeneous (at the end of first inner while loop): F :

$$\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

and the projection matrices become

$$Y = \begin{bmatrix} 2 & 1 & 3 & 3 \\ 2 & 2 & 1 & 3 \\ 2 & 2 & 2 & 1 \\ 3 & 2 & 2 & 2 \end{bmatrix} \ and \ X = \begin{bmatrix} 3 & 3 & 2 & 1 \\ 1 & 2 & 2 & 2 \\ 2 & 2 & 1 & 3 \\ 3 & 3 & 1 & 2 \end{bmatrix}$$

Make X as diagonally homogeneous (at the end of second inner while loop): F :

$$\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}$$

$$\begin{bmatrix} 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

and the projection matrices become

$$Y = \begin{bmatrix} 2 & 1 & 1 & 1 \\ 2 & 2 & 1 & 2 \\ 1 & 1 & 2 & 1 \\ 1 & 1 & 1 & 2 \end{bmatrix} \ and \ X = \begin{bmatrix} 1 & 2 & 2 & 1 \\ 0 & 1 & 2 & 2 \\ 2 & 0 & 1 & 2 \\ 3 & 2 & 0 & 1 \end{bmatrix}$$

Make Y as diagonally homogeneous (at the end of first inner while loop): F :

$$\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 1 \\ 1 & 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}$$

$$\begin{bmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

and the projection matrices become

$$Y = \begin{bmatrix} 2 & 1 & 1 & 1 \\ 1 & 2 & 1 & 1 \\ 1 & 1 & 2 & 1 \\ 1 & 1 & 1 & 2 \end{bmatrix} \ and \ X = \begin{bmatrix} 1 & 2 & 2 & 0 \\ 0 & 1 & 2 & 2 \\ 2 & 0 & 1 & 2 \\ 2 & 2 & 0 & 1 \end{bmatrix}$$

Make X as diagonally homogeneous (at the end of second inner while loop): Since X is already diagonally homogeneous, output of the previous step becomes the output of present step. F :

$$\begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 1 \\ 1 & 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}$$

$$\begin{bmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

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and the projection matrices become

$$Y = \begin{bmatrix} 2 & 1 & 1 & 1 \\ 1 & 2 & 1 & 1 \\ 1 & 1 & 2 & 1 \\ 1 & 1 & 1 & 2 \end{bmatrix} \; and \; X = \begin{bmatrix} 1 & 2 & 2 & 0 \\ 0 & 1 & 2 & 2 \\ 2 & 0 & 1 & 2 \\ 2 & 2 & 0 & 1 \end{bmatrix}$$

The bipartite graph G(left graph in fig2) and the sub graph of bipartite G such that flow value of every edge in the sub graph is 1(right graph namely network flow in fig.2.) are given in fig. 2. Note that G and G' are defined in Theorem 1.
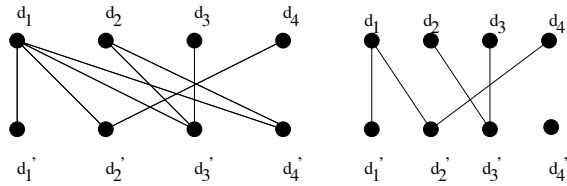

Fig. 2.   Bipartite Graph and Network Flow

The Mobile part: M :

$$\begin{bmatrix} 1 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix}$$

The reconstructed matrix: A :

$$\begin{bmatrix} 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix}$$

and the projection matrices become

$$Y = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \; and \; X = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

IV. Correctness

The algorithm $Fixed \; part$ finds the fixed $1'$ by considering the difference between adjacent row sums or column sums in the diagonal direction . For each fixed 1, the procedure Propagation fills F by periodicity $(1, \; 1, \; 1)$ and decreases the values in projection matrices.
At the end of $fixed \; part$ both projection matrices are

diagonally homogeneous, and at the end of procedure *make strong diagonal* both projection matrices become *strongly diagonally homogeneous*. By $lemma1$, mobile part can be constructed if max flow value is same as $\sum_{i=1}^{n} C(s, d_i)$, and there is no 3D-periodic matrix whose projection is equal to the given projection if max flow value is not same as $\sum_{i=1}^{n} C(s, d_i)$.

V. Complexity

The algorithm $Fixed \; part$ calls procedure $propagation$ $O(n^2)$ times, and each propagation does $O(n)$ operations. Hence Fixed part computation can be done in $O(n^3)$ operations. $make\_strong\_homogeneous$ procedure $O(n^2)$ operations. Since the number of vertices in graph G' defined in $Theorem1$ is $2n + 2$, the subgraph of the bipartite graph consists of edges whose flow value is 1 in G' can be computed in $O(n^3)$ by using max flow algorithm for the network G'[2] . Hence starting positions of all the loops are computed in $O(n^3)$ operations. Since the number of loops is $O(n)$ and loop() works in $O(n)$ times, placement of loops takes $O(n^2)$. Hence the time complexity of reconstruction algorithm is $O(n^3)$.

VI. Conclusion

In this paper we have extended the periodicity constraints to 3D-binary matrices. reconstruction of 2D-periodic matrices has been studied in [1]. As 3D-periodicity does not imply layer wise periodicity(2D-periodicity), the 3D-reconstruction is not straight forward. The similar greedy that works in 2D-problem to reconstruct mobile part does not work in 3D. We reduced the mobile part reconstruction problem to max flow problem and the solution of max flow problem is used to compute the mobile part of the reconstructed matrix. The motivation of this study is to reconstruct the crystal with periodicity constraints(natural constraints) so that the reconstructed crystal is not only has the same projection as that of unknown original crystalline structure, but also close to the unknown original crystalline structure. By considering periodicity constraints, the class of binary matrices representing the crystalline structure is reduced, and hence the reconstructed matrix is more close to unknown matrix. For instance, after fixed part computation if the projection matrices are zero matrices then unique solution is obtained.

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